

**Amendments to the Claims**

This listing of claims will replace all prior versions, and listings, of claims in the application:

**Listing of Claims**

1. (Currently Amended): A method for selecting at least one lead-candidate compound capable of binding as a ligand to a protein from a ~~compound~~ database ~~of trial compounds~~ comprising information on atomic types and covalent bonds of compounds in the database, comprising:
  - a) ~~choosing inputting~~ at least one query molecule that is known to bind, or expected to be capable of binding, to the protein; [[and]]
  - b) ~~selecting screening~~ lead-candidate compounds from the compound database by matching modes of covalent bonds between the query molecule and [a] ~~the trial compound compounds~~ stored in the database and judging similarity of partial structures of the query molecule and the trial ~~compound compounds~~ based on two-dimensional graphs of the query molecule and the trial compounds where each atom is represented as a node and each covalent bond is represented as an arc; and
  - c) ~~outputting at least one lead-candidate compound capable of binding to the protein.~~

2-5. (Cancelled)

6. (Currently Amended) The method of claim 1, wherein the compound database comprises information on three-dimensional structures of the trial compounds, and which wherein step (b) further comprises:

[[c]]) estimating a binding scheme of the lead-candidate compounds compound selected in step b) to the protein based on three-dimensional information and binding scheme of the query molecule to the protein of the query molecule and based on correspondence of the partial structures of the query molecule and the trial trial compound compounds;

[[d]]) calculating one or more parameters relating to interaction between the lead-candidate compounds compound and the protein; and

[[e]]) screening the lead-candidate compounds capable of binding as a ligand to the protein based on the parameters relating to interaction between the lead-candidate compounds and the protein calculated in step d).

7. (Currently Amended): The method of claim 1, wherein the compound database comprises information on three-dimensional structures of the trial compounds, and which wherein the step (b) further comprises:

[[c]]) estimating a virtual receptor model which represents physicochemical environment of the ligand binding site of the protein based on information of three-dimensional structures of one or more known ligands capable of binding to the protein;

[[d]]) fitting the lead-candidate compound selected in step b) to the virtual receptor model and judging goodness of fit of the trial compounds to the virtual receptor model; and

[[e]] screening the ~~trial~~ lead-candidate compounds capable of binding as a ligand to the protein based on the goodness of fit.

8-10. (Cancelled)

11. (Currently Amended) The method of claim 1, further comprising wherein step (a) further comprises constructing the structure of the at least one query molecule by an automatic structure construction method.

12. (Currently Amended) The method of claim 6, further comprising wherein step (a) further comprises constructing the structure of the at least one query molecule by an automatic structure construction method.

13. (Currently Amended) The method of claim 7, further comprising wherein step (a) further comprises constructing the structure of the at least one query molecule by an automatic structure construction method.